

Sebacic acid, 3-methylbut-3-enyl tetradecyl ester

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|----------------------|--|
| Inchi: | InChI=1S/C29H54O4/c1-4-5-6-7-8-9-10-11-12-15-18-21-25-32-28(30)22-19-16-13-14-17 |
| InchiKey: | ASEKKXCWQRPDLV-UHFFFAOYSA-N |
| Formula: | C29H54O4 |
| SMILES: | C=C(C)CCOC(=O)CCCCCCCC(=O)OCCCCCCCCCCCCC |
| Mol. weight [g/mol]: | 466.74 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -195.25 | kJ/mol | Joback Method |
| hf | -1015.85 | kJ/mol | Joback Method |
| hfus | 73.85 | kJ/mol | Joback Method |
| hvap | 97.87 | kJ/mol | Joback Method |
| log10ws | -9.54 | | Crippen Method |
| logp | 8.861 | | Crippen Method |
| mcvol | 430.050 | ml/mol | McGowan Method |
| pc | 670.12 | kPa | Joback Method |
| rinpol | 3257.00 | | NIST Webbook |
| tb | 1012.06 | K | Joback Method |
| tc | 1258.72 | K | Joback Method |
| tf | 545.19 | K | Joback Method |
| vc | 1.690 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1508.79 | J/mol×K | 1012.06 | Joback Method |
| cpg | 1531.49 | J/mol×K | 1053.17 | Joback Method |
| cpg | 1552.14 | J/mol×K | 1094.28 | Joback Method |
| cpg | 1570.83 | J/mol×K | 1135.39 | Joback Method |
| cpg | 1587.66 | J/mol×K | 1176.50 | Joback Method |
| cpg | 1602.71 | J/mol×K | 1217.61 | Joback Method |
| cpg | 1616.09 | J/mol×K | 1258.72 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U355945&Units=SI |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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